Argonne NATIONAL LABORATORY

ESP Kick-Off Workshop
Project Plan Presentation

High Speed Combustion and Detonation

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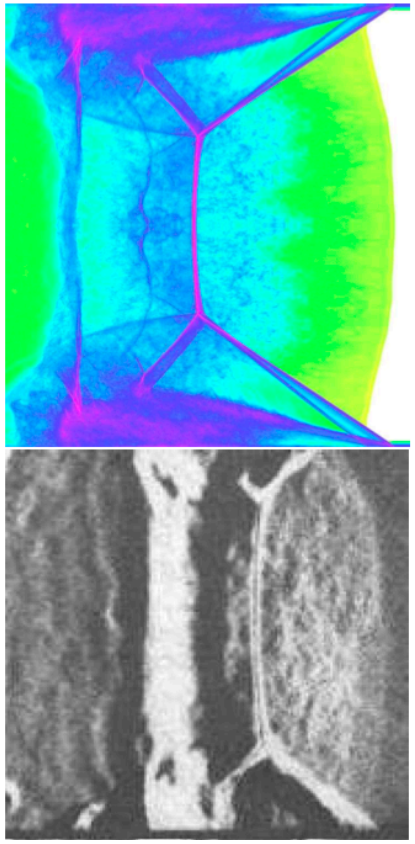
Project Overview

Understanding the detonation-to-deflagration transition (DDT) in hydrogen.

- **Enable commercial use of hydrogren fuel**
  - Mira allows first simulations at real scale and real Reynolds number 10^7. Intrepid only allows Reynolds number 10^5.



Scientific Field: Combustion

Codes: FTT/ALLA

Computational Approach, Numerical Methods

- **Reactive Navier-Stokes direct numerical simulation**
  - equation of state (EOS), microscopic transport, and chemical kinetics suitable for hydrogen combustion
  - Euler fluxes are calculated using a second-order accurate, Godunov-type, conservative scheme with a Riemann solver [13] and a monotone VanLeer reconstruction [12].
  - Viscous, mass diffusion, and heat fluxes are calculated using second-order central differencing.
- **Adaptive Mesh Refinement**
  - Fully Threaded Tree, all tree operations parallel
  - 2.6 integers per cell, less than oct-tree or threaded oct-tree
- **We use the sound crossing time Courant stability criterion because it is more stringent than stability criteria for integrating parabolic-type Navier- Stokes terms with numerical resolution of the DNS DDT calculations of interest.**

Parallelism and Existing Implementation

- Mesh distributed across MPI ranks using Morton ordering
- Adaptive mesh refinement and rebalancing every four timestep
- MPI plus OpenMP in physics/chemistry
- I/O: Using MPI-IO collectives

Library and Tool Dependencies

- **Libraries**
  - No external libraries
- **Tools**
  - Fttv for 2-D viz, VISIT for 3-D viz

Anticipated Modifications for Blue Gene/Q

- **Improved load-balancing**
  - Current scheme starts to fail at 32K MPI ranks
- **Improved I/O, possibly in a background thread**
  - Current OpenMP scaling is 3.3x for 4 threads; could sacrifice one thread to skip checkpoint steps
  - Current memory/rank supports keeping a copy of the data to dump
- **Automatic visualization of physics regions of interest**

Plan for Next 6 Months Effort

- **Hire a postdoc**
- **Work on 3-D visualization through VISIT/VTK**
- **Work on I/O dump speed**